PH 5840 Lectures - 5, 6

Note Title 8/10/2015

Density Operator: ρ is associated with an ensemble of states $\{p_i, |\psi_i\rangle\}$ iff $\rho \geq 0$, $Tr(\rho) = 1$.

Proof: Let $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$.

Then, $Tr(\rho) = \sum_i p_i \langle\psi_i|\psi_i\rangle = 1$

$$\langle\phi|\rho|\phi\rangle = \langle\phi|\left(\sum_i p_i |\psi_i\rangle\langle\psi_i|\right)|\phi\rangle$$

$$= \sum_i p_i |\langle\phi|\psi_i\rangle|^2 \geq 0, \ \forall |\phi\rangle.$$

Conversely, let $\rho \geq 0$, $Tr(\rho) = 1$.

spectral decomposition: $\rho = \sum_i \lambda_i |i\rangle\langle i|$

$\Rightarrow$ Ensemble of states $\{\lambda_i, |i\rangle\}$

QED

(i) Pure vs. Mixed states:

$$\left.\begin{array}{l} |\psi\rangle \longleftrightarrow |\psi\rangle\langle\psi| \ \text{rank-1 projector} \\ Tr\left((|\psi\rangle\langle\psi|)^2\right) = Tr(|\psi\rangle\langle\psi|) = 1 \end{array}\right\} \text{Pure state}$$

In general, $Tr(\rho^2) < Tr(\rho) = 1$

$\Rightarrow \rho$ is mixed.

* $Tr(\rho^2) = 1$ if and only if ρ is a pure state.

② Ensemble corresponding to a density matrix is not unique :-

(Eg 1) Consider $\rho = \frac{3}{4}|0\rangle\langle 0| + \frac{1}{4}|1\rangle\langle 1|$

$$\text{Let } |a\rangle = \sqrt{\frac{3}{4}}|0\rangle + \sqrt{\frac{1}{4}}|1\rangle$$

$$|b\rangle = \sqrt{\frac{3}{4}}|0\rangle - \sqrt{\frac{1}{4}}|1\rangle$$

Then $\rho' = \frac{1}{2}|a\rangle\langle a| + \frac{1}{2}|b\rangle\langle b|$

$$= \frac{3}{4}|0\rangle\langle 0| + \frac{1}{4}|1\rangle\langle 1| \equiv \rho \; !$$

$$\rho \equiv \left\{\frac{3}{4}|0\rangle, \frac{1}{4}|1\rangle\right\} \equiv \left\{\frac{1}{2}|a\rangle, \frac{1}{2}|b\rangle\right\}$$

③ SHJW Theorem: How are different ensembles corresponding to the same density operator related?

Two ensembles $\{p_i, |\psi_i\rangle\langle\psi_i|\}$ and $\{q_j, |\phi_j\rangle\langle\phi_j|\}$ generate the same density matrix ρ if and only if

$$\sqrt{p_i}\,|\psi_i\rangle = \sum_{j=1}^{m} u_{ij}\sqrt{q_j}\,|\phi_j\rangle, \quad \forall i=1,2,\ldots n$$

where $u_{ij} \equiv U$ is a $p \times p$ unitary matrix, where, $p = \max(n,m)$

Note: We append zero vectors to the ensemble with fewer states, so both $\{|\tilde{\psi}_i\rangle = \sqrt{p_i}|\psi_i\rangle\}$ and $\{|\tilde{\phi}_j\rangle = \sqrt{q_j}|\phi_j\rangle\}$ have the same number ('p') of states.

Proof:

(i) Let $|\tilde{\psi}_i\rangle = \sqrt{p_i}\,|\psi_i\rangle$, $|\tilde{\phi}_j\rangle = \sqrt{q_j}\,|\phi_j\rangle$.

Given, $|\tilde{\psi}_i\rangle = \sum_{j=1}^{p} u_{ij}|\tilde{\phi}_j\rangle$ where $u_{ij} = U$ is unitary.

Then, $$\sum_i |\tilde{\psi}_i\rangle\langle\tilde{\psi}_i| = \sum_i \sum_{j,k} u_{ik}^* u_{ij} |\tilde{\phi}_j\rangle\langle\tilde{\phi}_k|$$
$$= \sum_{j,k} \underbrace{\sum_i (U^\dagger)_{ki}(U)_{ij}}_{\delta_{jk}} |\tilde{\phi}_j\rangle\langle\tilde{\phi}_k|$$
$$= \sum_j |\tilde{\phi}_j\rangle\langle\tilde{\phi}_j| = \rho$$

Conversely:-

Given, $\sigma = \sum_i |\tilde{\psi}_i\rangle\langle\tilde{\psi}_i| = \sum_j |\tilde{\phi}_j\rangle\langle\tilde{\phi}_j|$ —①

Spectral decomposition: $\sigma = \sum_{k=1}^{r} \lambda_k |e_k\rangle\langle e_k|$ —②

'r' is the rank of ρ

Let $|f\rangle$ be a vector $\perp^r$ to the span of $\{|e_k\rangle\}$.

Then, $\langle f|\sigma|f\rangle = 0 = \sum_i \langle f|\tilde{\psi}_i\rangle\langle\tilde{\psi}_i|f\rangle$

$\sum_i |\langle\tilde{\psi}_i|f\rangle|^2 = 0$ (sum of positive terms!)

$\Rightarrow |\langle\tilde{\psi}_i|f\rangle| = 0$, $\forall\, i = 1,2,\dots n$.

$\therefore$ $(\forall i=1,2,\dots n)$, $|\tilde{\psi}_i\rangle = \sum_{k=1}^{r} c_{ik}|\tilde{e}_k\rangle$ $(|\tilde{e}_k\rangle = \sqrt{\lambda_k}\,|e_k\rangle)$

$(c_{ik} = C$ is a $n\times r$ matrix$)$

Let $s = \max(n,r)$. Appending zero-vectors to the smaller set, we have,

$$|\tilde{\psi}_i\rangle = \sum_{k=1}^{s} v_{ik}|\tilde{e}_k\rangle,\ i=1,2,\dots,s \quad \text{—③}$$

where $v_{ik} = V$ is a $s\times s$ matrix, with additional rows or columns added to C, to make it square | $V = \begin{pmatrix} \underbrace{\quad C \quad}_{r} \big\updownarrow n \end{pmatrix}_{s \times s}$

Substituting ③ in ① or ②, we get

$$\sum_{i,k,l=1} v^*_{il} \, v_{ik} \, |\tilde{e}_k\rangle\langle\tilde{e}_l| = \sum_{m=1}^{s} |\tilde{e}_m\rangle\langle\tilde{e}_m|$$

> **Note:** Operators $|\tilde{e}_k\rangle\langle\tilde{e}_l|$ are linearly independent.
>
> i.e. If $\sum_{k,l} c_{kl} \, |\tilde{e}_k\rangle\langle\tilde{e}_l| = 0$
>
> then $c_{kl} = 0 \;\; \forall \; k, l$.
>
> "Proof": $\left(\sum_{k,l} c_{kl} \, |\tilde{e}_k\rangle\langle\tilde{e}_l|\right) |\tilde{e}_i\rangle = 0$
>
> $$\Rightarrow \sum_k c_{ki} \, |\tilde{e}_k\rangle = 0$$
>
> $$\Rightarrow c_{ki} = 0 \;\; \forall \; k$$ since $\{|\tilde{e}_k\rangle\}$ are linearly independent.

$\therefore \; \sum_{i=1}^{s} v^*_{il} \, v_{ik} = \delta_{lk} \;\Rightarrow\; v_{ik} \equiv V$ is a $s \times s$ unitary matrix.

Ill'ly $|\tilde{\phi}_j\rangle = \sum_{k=1}^{t} w_{jk} \, |\tilde{e}_k\rangle \;\Rightarrow\; w_{jk} \equiv W$ is a $t \times t$ unitary matrix.

where $t = \max(m, r)$.

$$\Rightarrow \sum_j w^*_{jl} \, |\tilde{\phi}_j\rangle = \sum_{k,j} w^*_{jl} \, w_{jk} \, |\tilde{e}_k\rangle = |\tilde{e}_l\rangle \quad \text{—— ④}$$

Putting together ③ and ④, we have,

($p = \max(s,t)$, append zero-vectors to the smaller set again!)

$$|\tilde{\psi}_i\rangle = \sum_{k=1}^{p} v_{ik} |\tilde{e}_k\rangle$$

$$= \sum_{k=1}^{p} \sum_{j=1}^{p} v_{ik} w_{jk}^{*} |\tilde{\phi}_j\rangle$$

$$= \sum_j \sum_k (V)_{ik} (W^{\dagger})_{kj} |\tilde{\phi}_j\rangle$$

$$= \sum_j u_{ij} |\tilde{\phi}_j\rangle$$

where $(U)_{ij} = \sum_{k=1}^{p} (V)_{ik} (W^{\dagger})_{kj}$

i.e. $U = VW^{\dagger}$ is also a $p \times p$ unitary!

× ——— × ——— × ——— ×

④ Revisiting the postulates of Q. mech :-

(a) State of a system is a positive operator of unit trace (trace-class)

$$\rho \in S(\mathcal{H}) \subseteq \mathcal{B}(\mathcal{H}) \subseteq \mathcal{L}(\mathcal{H})$$

(b) Dynamics : $\rho(t) = U(0,t)\, \rho(0)\, U^{\dagger}(0,t)$

(c) Measurement : $M = \{M_i\}$

$$p(i) = \mathrm{Tr}(\rho M_i)$$

$$\rho \longrightarrow \sum_i M_i \rho M_i^{\dagger}$$